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Electrons in and close to Correlated Systems

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ELECTRONS

IN AND CLOSE TO CORRELATED SYSTEMS

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Preface

The electronic structure of solids which are influenced by electron-electron interactions is an important field of study, both theoretical and experimental. This is certainly supported by the interesting properties of the materials in which electron correlation effects are a prerequisite to describe their electronic properties. Important examples are the high temperature superconductors, the transition metal oxides and the Kondo systems. Information on effects derived from electron correlation can be obtained from several experimental studies, among which spectroscopic techniques that measure the momentum dependent energy distribution of scattered or emitted electrons. The development and installation of a new high resolution electron spectroscopy system with which such studies can be performed at arbitrary scattering geometries, was the main assignment for my graduate work in the group of Prof. G.A. Sawatzky at the University of Groningen.

In this thesis called:

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phenomena will be discussed which are strongly dependent on momentum, defined by a combination of the electron energy and the detection angle relative to the surface normal. Contrary to results obtained by the use of optical techniques, in electron spectroscopic results large possibilities are offered by selection of the momenta of the probing electrons and/or of the detected electrons. For example measurements of dispersion relations. The momentum of the electrons in combination with the reciprocal lattice of the surface under study can however influence much more than is generally realized. This in reference to diffraction effects and symmetry induced effects in the probed electronic structure. The processes that will be discussed have a fundamental character and will possibly lead to new directions in electron spectroscopic studies.

The propagation of electrons and holes *IN* systems with an electronic structure determined by electron-electron interactions, so called correlated systems, are extensively studied. Numerous angle resolved ultraviolet photoemission spectroscopy(ARUPS) studies have been performed on correlated systems, especially the transition metal oxides and the transition metal oxide based compounds, like the cuprate systems. In the case of the cuprates the spectral region near the Fermi energy resembles the strongly hybridized character of the compounds. Weak "quasiparticle"-like features are observed which originate from Zhang-Rice singlet derived states, a state formed by a combination of Cu and O orbitals which results in maximum overlap and so in a maximum mixed state. The dispersion

of these strongly hybridized singlets can be studied as a function of doping of the CuO_2 plane with electrons or holes. As such, possible features originating from the same orbitals as the Zhang-Rice singlets, but this time forming a combination that results in minimum mixing, could act as a reference point between spectra at all doping levels as insensitivity to the doping level is expected.

Processes taking place in a region outside but *CLOSE* to single crystalline surfaces can result in features within the same photoemission spectra as the ones discussed above. When the combination of detection angle, photon energy and orientation of the crystal is "unfortunately" chosen, electrons with fixed kinetic energies can interfere with the spectral features of interest. Electron Energy Loss Spectroscopy(EELS) is well suited to study these conditions both directly and indirectly injected. On the basis of EELS results on a variety of surfaces the origin will be discussed. The influences on elastic scattering intensities and on the observation of elementary excitations will be examined.

These briefly mentioned phenomena will be studied in detail in the following Chapters. In Chapter I the characteristics of the developed electron spectroscopy system will be discussed in combination with the basic theory of it's two main applications; EELS and ARUPS. Some of the aspects of electron correlation will be introduced in Chapter II, this will serve as a theoretical background for the excitations studied in the rest of this thesis. In Chapter III pre-emergent Bragg diffraction is introduced as the origin of strong resonances in energy loss experiments and constant kinetic energy features in techniques like photoemission and secondary electron spectroscopy. The principle of such waveguide behaviour can be used in studies on elementary excitations. On the basis of an extensive energy loss study on NiO(100), waveguide related enhancement effects of in this case *d*-*d* excitons and surface optical phonons will be shown in Chapter IV. The dynamics of the propagation of a (single) hole inside the CuO_2 plane at half filling will be discussed in Chapter V. This data will be used to demonstrate that the hybridization in strongly correlated systems is not constant in momentum space. As such it can happen that features unrecognizable throughout most of the Brillouin zone become very intense and narrow at selected conditions. Peaks observed at high symmetry points only, are proposed to originate from states that have no copper character, to be independent of doping and to be useful as a reference point in doping dependent photoemission studies. In Chapter VI the theoretical influence of the lower symmetry at the surface relative to the bulk, on the Madelung potential and as a direct result on the conduction gap will be discussed.

To make reading of this thesis easier a List of Figures is added as some figures are referred to at multiple positions in the text.

Hans Pothuizen

Groningen, 1998.

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